Computer-Aided Engineering and Next Generation Development of Electric Drive Batteries

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1. Background & Penn State Battery R&D
2. Computer-Aided Engineering of xEV Batteries
3. Next Generation of xEV Batteries
4. Summary
Electrochemical Engine Center

- Founded in 1997
- Engaged in battery and fuel cell research for vehicle electrification
Lithium-Ion Battery Manufacturing Facility
Energy Storage Technologies for a Sustainable Future

- Batteries for: PHEV, renewable energy storage, smart grids, etc.

- All-day power for iPhones, iPads, iPods, wireless society
President Obama visits Penn State University and speaks about encouraging and investing in innovation and clean energy technologies to create new jobs, grow the economy, and win the future.

Penn State: #1 ranking in alternative energy among universities globally (Elsevier, 2010)
Penn State: #1 ranking in fuel cells among universities worldwide (ScienceWatch, 2009)
Penn State: one of only 3 Energy Hubs ($129M in Energy Efficient Buildings)
Net-Zero Energy Building
Computer-Aided Engineering of Batteries

Materials Characterization
Physico-chemical Modeling
Computational Algorithms
Diagnostics & Validation

Set **Gold Standard** for Vehicle Battery Engineering

Performance
Cycle Life
Safety

- highest active material utilization
- highest energy density (Wh/kg)
- longest life
- lowest life-cycle cost
- lowest cost $/kWh
- safest systems by virtual & actual testing
Evaluating Various Designs

**Single-Jelly Roll Design**
- t=100s
- t=3500s

**Multi-Jelly Roll Design**
- t=100s
- t=3500s

**Stacked Electrode Design**
- t=100s
- t=500s

**1C discharge current distribution**
- Electrode length (cm)
- Current density (mA/cm²)

**6C discharge current distribution**
- Electrode length (cm)
- t=100s
- t=500s
• Ensuring current distribution uniformity (and hence uniformly high utilization of active materials) quantitatively impacts the cell’s energy density (by as much as 50%)
• It is as significant as developing advanced Li-ion chemistries or going beyond Li-ion! In addition, it makes immediate commercial advances!
Cycle Life – Key to EV Commercialization

• battery cycle life is a major challenge
• directly impacts warranty and hence cost
• very time-consuming and expensive information
• computer simulation ~500x faster than real testing time, e.g.
  ➢ for 6-min pulsed power cycle, simulation ~ 1 s
  ➢ for 1h charge/discharge, simulation ~ 10 s
  ➢ for 6-12 months cycle life testing, simulation ~ 12-24 hrs

10% error in life prediction results in 50% cell failure before expiration of warranty.
LFP cell cycled @ C/2 between 2.0-3.6V
Cycle Life Prediction & Exp. Validation – NMC-Gr Chemistry

25°C 1C characterization

25°C 2C characterization

25°C 5C characterization

25°C 10C characterization

50°C 5C cycling

Capacity (mAh)

Cell Voltage (V)

Temperature (°C)

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Predicting Battery SOH at Various T and C-rate

LFP-Gr
Cycle life is significantly shortened by elevated temperature: ~2,000 cycles at RT but <1,000 cycles at 45°C. This indicates the paramount importance of thermal management for battery pack life extension.

SOH = capacity of aged cell/initial capacity (nominal)
- Cost to Boeing of reimbursing airlines for the lost revenue due to Li-ion safety-related grounding of 787 was $550M*
- As Li-ion batteries become more energy dense (smaller), potential for catastrophic safety incident increases
Active material thermal stability is NOT equal to battery safety. The latter is an integrated result of SEI layer stability, electrolyte stability, & anode/cathode material stability, as well as cell structure.

Thermal runaway experiment
Nail Penetration & Internal Short

Full Nail Penetration

More uniform heat generation

Current on tabs

Precipitous T rising due to small tabs

Partial Nail Penetration

No current on tabs

Current Collector (Cu)

Current Collector (Al)

Internal Short

Metal Particle

Negative Electrode

Separator

Positive Electrode
Full and partial penetration

**Full Penetration**

Maximum temperature during shorting event ($^\circ$C)

- Diameter = 0.5 mm
  - Tmax = 180$^\circ$C
  - Tavg = 53$^\circ$C
  - Tmax-Tavg = 127$^\circ$C

- Diameter = 8 mm
  - Tmax = 58$^\circ$C
  - Tavg = 53$^\circ$C
  - Tmax-Tavg = 5$^\circ$C

**Separator shutdown**

- Separator shutdown ineffective
- Separator shutdown effective

**Partial Penetration**

Maximum temperature ($^\circ$C)

<table>
<thead>
<tr>
<th>Nail penetration depth</th>
<th>0.1s</th>
<th>0.5 s</th>
<th>1.0 s</th>
<th>5.0 s</th>
<th>20 s</th>
</tr>
</thead>
<tbody>
<tr>
<td>Anode</td>
<td>170.3</td>
<td>160.0</td>
<td>149.6</td>
<td>139.2</td>
<td>128.8</td>
</tr>
<tr>
<td>Separator</td>
<td>118.4</td>
<td>108.1</td>
<td>97.69</td>
<td>87.31</td>
<td>76.93</td>
</tr>
<tr>
<td>Cathode</td>
<td>46.55</td>
<td>56.17</td>
<td>45.79</td>
<td>35.94</td>
<td>25.94</td>
</tr>
</tbody>
</table>

**Nail penetration depth (normalized by cell thickness)**

- 0.1 s
- 0.5 s
- 1.0 s
- 5.0 s
- 20 s

**Nail diameter (mm)**

- 0.5
- 8

**Separator shutdown ineffective**

- Effective
- Ineffective
Internal short

Internal Short \( (R_{\text{short}} = 10 \text{ milliohms}) \)

Surface temperature

- 0.1s
- 5s
- 40s
- 80s

Internal temperature

- 0.1s
- 5s
- 40s
- 80s

Voltage (V) vs. Time (sec)

Current (C-rate) vs. Time (sec)

Temperature (°C) vs. Time (sec)

Graphs showing the changes in surface and internal temperatures over time, along with voltage, current, and temperature graphs.
Enhanced Module/Pack Safety

Cells: 35Ah, 4P
AM: Graphite/NMC
Cooling: Liquid
Cell 1 nail-penetrated

Loss of coolant w/ coolant

Time[s]
0 100 200 300 400

Tmax[°C]
25 75 125 175 225 275 325 375 425

w/o coolant
w/ coolant

T (°C)
127 116 105 94 83 72 61 50 39

T (°C)
62 57 52 47 42 37 32 27
Overcharge: Effect of Cathode Material

- Cathode material has dramatic effect on overcharge behavior. LFP is less tolerant to overcharge.
- Significant overcharge of LFP battery even at 1C leads to thermal runaway.

BYD e6 taxi (powered by LFP batteries) caught fire on 6/20/2013 at charging station in Hong Kong.

- Cell: NCM 20 Ah, LFP 20 Ah
- Thermal condition: Adiabatic
- Charge current: 1C, 10C
• Driving range per charge solely depends on energy density of batteries; 300-mile batteries are desirable.

Li-S Battery for Transportation Energy Storage

![Graph comparing energy density of different battery types: Lead-Acid, Ni-Cd, Ni-MH, Li-Ion, Li-S, Zinc-Air, Li-Air, and Gasoline. The theoretical and practical energy densities are shown in blue and orange bars, respectively. The highest theoretical and practical energy densities are for Gasoline at 1700 Wh/Kg.]
Li-S Battery

<table>
<thead>
<tr>
<th>cathode</th>
<th>theoretical capacity (mAh/g)</th>
<th>electrode voltage</th>
<th>actual capacity (mAh/g)</th>
<th>estimated price ($)</th>
</tr>
</thead>
<tbody>
<tr>
<td>LiCoO₂</td>
<td>275</td>
<td>3.7</td>
<td>130-140</td>
<td>1</td>
</tr>
<tr>
<td>LiNiO₂</td>
<td>274</td>
<td>3.4</td>
<td>170-180</td>
<td>0.86</td>
</tr>
<tr>
<td>LiMn₂O₄</td>
<td>148</td>
<td>3.8</td>
<td>100-120</td>
<td>0.17</td>
</tr>
<tr>
<td>V₂O₅</td>
<td>400</td>
<td>2.5</td>
<td>120-200</td>
<td></td>
</tr>
<tr>
<td>S₈</td>
<td>1672</td>
<td>2.1</td>
<td>&gt;1000</td>
<td>0.017</td>
</tr>
</tbody>
</table>

- Issues: polysulfide shuttle effect after dissolution, resulting in low efficiency, low active material utilization; low electronic conductivity
- Solutions: absorbents, electrolyte additives, graphene fillers, etc.
80% capacity retained in 100 cycles
77% capacity retained in 170 cycles
Li-S Cell Performance @ C/2 Rate

75% capacity retained in 100 cycles
70% capacity retained in 300 cycles
Summary

• Current Generation Li-ion Battery for Vehicle Electrification:
  – Specific Energy or Energy Density: 200 Wh/kg or 400 Wh/L
  – Cycle Life: >5000
  – Cost (@ Cell Level): <$150/kWh
  – High Safety: ~60Ah Cells and large packs still safe
  – CAE of vehicle batteries is a main tool to achieve all above.

• Beyond Li-ion:
  – Li-S battery for 300+ mile range
  – 2x or 3x energy density of current LiB
  – potentially low-cost
  – has achieved 1,000 mAh/g after 200 cycles in coin cells
  – prototyping in 1-10Ah being pursued.
Acknowledgements